

Cs_{0.9}Lu₃F_{9.9}*hP*15(187) *P*-6*m*2 – k³jha**Cs_{0.9}Lu₃F_{9.9}** [1]

Structural features: LuF₇ pentagonal bipyramids share edges and vertices to form a 3D-framework; Cs in channels parallel to [001].

Marsh R.E. (1986) [1]

Cs_{0.90}F₁₀Lu₃*a* = 0.7943, *c* = 0.4227 nm, *c/a* = 0.532, *V* = 0.2310 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	3 <i>k</i>	<i>mm</i> 2	0.165	0.835	¹ / ₂		
Lu2	3 <i>k</i>	<i>mm</i> 2	0.49136	0.50864	¹ / ₂		
F3	3 <i>k</i>	<i>mm</i> 2	0.7828	0.2172	¹ / ₂		non-colinear Lu ₂
F4	3 <i>j</i>	<i>mm</i> 2	0.5139	0.4861	0		non-colinear Lu ₂
F5	2 <i>h</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.381	0.5	
Cs6	1 <i>a</i>	-6 <i>m</i> 2	0	0	0	0.9	trigonal prism F ₆

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.024

Remarks: Supersedes a refinement in space group (8) *Cm* in [2] (~Cs_{0.75}Lu₃F_{9.75}), which does not take into consideration all symmetry elements; refinement on the same diffraction data. Short interatomic distances for partly occupied site(s).

References: [1] Marsh R.E. (1986), J. Solid State Chem. 64, 119-121. [2] Metin J., Chatonier D., Avignant D., Chevalier R., Cousseins J.C. (1984), J. Solid State Chem. 55, 299-305.